Connectivity-dependent properties of diluted sytems in a transfer-matrix description

S. L. A. de Queiroz[a*] and R. B. Stinchcombe[b†]
[a] *Instituto de Física, Universidade Federal Fluminense, Avenida Litorânea s/n, Campus da Praia Vermelha, 24210-340 Niterói RJ, Brazil*
[b] *Department of Physics, Theoretical Physics, University of Oxford, 1 Keble Road, Oxford OX1 3NP, United Kingdom*

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We introduce a new approach to connectivity-dependent properties of diluted systems, which is based on the transfer-matrix formulation of the percolation problem. It simultaneously incorporates the connective properties reflected in non-zero matrix elements and allows one to use standard random-matrix multiplication techniques. Thus it is possible to investigate physical processes on the percolation structure with the high efficiency and precision characteristic of transfer-matrix methods, while avoiding disconnections. The method is illustrated for two-dimensional site percolation by calculating (*i*) the critical correlation length along the strip, and the finite-size longitudinal DC conductivity: (*ii*) at the percolation threshold, and (*iii*) very near the pure-system limit.

The transfer-matrix (TM) approach to percolation was pioneered by Derrida and coworkers [1]. By analysing the possible combinations of adjacent column states made up of occupied and unoccupied sites (or bonds), and the allowed connections among the latter and to the arbitrary origin of a two-dimensional ($d = 2$) strip, it was possible to write the TM on the basis of such column states. The key element in this formulation was the fact that, from the very structure of the TM, repeated multiplication is tantamount to the simultaneous generation of all possible connected configurations that span the strip, each with its proper probabilistic weight. Thus the probability of connection to the origin, whose exponential decay is governed by the correlation length, is asymptotically given exactly by the largest eigenvalue of the TM. The correlation length could then be used in a phenomenological renormalisation calculation [2], which gave very accurate results for critical parameters such as the percolation threshold and correlation-length exponent ν. It was not clear, however, how one could take advantage of such a direct and elegant scheme to investigate properties other than the decay of the probability of connection to the origin. The obvious alternative, of building up successive columns by occupying (or not) each individual site independently, runs into the problem of disconnections, which is severely aggravated on a strip geometry. Up to now, the usual solution has been to generate configurations site by site, and study quantities which do not depend on keeping connectivity along the strip, *e.g.* the moments of the distribution of clusters [3] for percolation in $d = 2$ and 3. A clever way to get round the effects of disconnections for random resistor-insulator networks at percolation was introduced [4] by generating individual elements on long strips (or bars, in $d = 3$) with *free* edges. By imposing a fixed voltage drop *across* the strip, it was possible to invoke TM concepts in a step-by-step evaluation of the transverse conductivity, for which longitudinal disconnections of the resistor structure are irrelevant. Finally, in superconductor-resistor networks at the percolation threshold of superconducting elements, disconnections are in fact responsible for the quantity of interest, which is the residual finite-size resistivity; one can then establish periodic boundary conditions across the strip (in order to minimise finite-width effects) and estimate the longitudinal resistivity [5,6].

Here we introduce a scheme which preserves the connected structure of the percolating cluster as one sweeps along the strip, and at the same time relies on standard ideas of random-matrix multiplication. The latter feature implies that any physical quantity, in addition to connection probability, can be sampled along the strip through insertion of its corresponding local realisation. This opens the way *e.g.* to the straightforward treatment of spin-spin correlations in dilute magnets [7], for which so far only approximate TM treatments, relying on plausible but essentially uncontrollable assumptions, have been available [8]. In the new scheme we enumerate the set of all allowed column combinations, according to the original TM procedure [1], and then build the strip one full column at a time, by picking a given column's successor at random but *only among those columns that are allowed* by the connectivity rules (*i.e.*, which have a non-zero TM element linking them to the immediate predecessor). With the proper assignment of probabilistic weights, as explained below, this procedure is equivalent to the sampling of connected configurations implicit in the iteration of the TM.

In what follows, we first expose the basic concepts of the method; then the decay of correlations is calculated and shown to reproduce the results given by diagonalisation of the TM. Next we apply the method to the longitudinal conductivity of a diluted resistor-insulator

network. For this particular process high-accuracy results exist, together with some exact ones, which provide a test of the method. At the percolation point, the new method produces estimates of the conductivity exponent which compare very favourably with those existing in the literature. Near the pure-network limit, we obtain the corrections to the conductivity to first order in defect concentration, in excellent numerical agreement with analytical results. Finally we point to possible extensions and generalisations of the present approach.

We consider a strip of a square lattice of width L sites, with periodic boundary conditions across, on which sites may be independently occupied (unoccupied) with probability p $(1-p)$. As explained in Ref. [1], one builds all possible column configurations in which at least one site is occupied *and* linked to the origin (assumed to be at the far left, say); other sites may be either occupied and connected, occupied and disconnected, or unoccupied. The TM element T_{ij} between column configurations i and j is non-zero only if column j is allowed to succeed column i (meaning: connection to the origin must be preserved, and illogical situations, such as an occupied and disconnected site being preceded by a connected one on the same row, must not occur). One has

$$T_{ij} = p^{N_j} (1-p)^{L-N_j} \quad , \tag{1}$$

where N_j is the number of occupied sites in j. Our procedure then goes as follows. Assume that the strip has been built up to a column whose configuration is i. Call $\{j(i)\} \equiv j_1, j_2, \dots j_{M_i}$ the set of all j's (a total of M_i) allowed to succeed a given i. A segment of length

$$L_i = \sum_{\{j(i)\}} L_{ij} = \sum_{\{j(i)\}} p^{N_j} (1-p)^{L-N_j} \tag{2}$$

represents the total (conditional) probability to have a connected configuration succeeding column i. Drawing a random number $0 < \epsilon < 1$ from a uniform distribution, the next column configuration is chosen to be j_{i_0} such that

$$\sum_{j=j_1}^{j_{i_0-1}} L_{ij} < \epsilon L_i < \sum_{j=j_1}^{j_{i_0}} L_{ij} \quad . \tag{3}$$

This ensures that the allowed connected configurations come up with their proper corresponding probabilities. One can then proceed and generate a column to succeed j_0, and so on iteratively. The only information to be kept in store throughout the process is the same as that used in the standard TM formalism: the location and indices (column occupancy numbers) of non-zero TM elements.

We now show that for a strip of width L, the scheme described above gives the same correlation length, ξ_L, as that obtained from diagonalisation of the TM. One defines $\xi_L(p)$ through the exponential decay of the probability of connection between columns 0 and N, $P_N(p)$:

$$P_N(p) \sim \exp(-N/\xi_L(p)) \quad . \tag{4}$$

As the process described here is a *sequential sampling* one (as opposed to the parallel updating of mutually excluding paths in configuration space, which takes place in the iteration of the TM), one must consider the appropriate quantities to analyse. At each step, when column configuration j_{i_0} is chosen among M_i to succeed i, one is probing one branch of a tree structure in the space of column configurations, and discarding $M_i - 1$ others. In order to deal with this, and produce unbiased samples, the standard procedure is the weighting of steps introduced in early simulations of self-avoiding walks [9]. When considering the allowed moves from a point i to the next (here: in configuration space, as opposed to real space in Ref. [9]) one generates a weight W_i proportional to the total probability of moving out from that point. In the present case, $W_i = L_i$ of Eq. (2). It is easy to see that W_i is properly normalised, as the denominator is the sum of probabilities of *all* possible succeeeding configurations, not only connected ones, and that is unity. The total weight of a given $N-1$- step walk (spanning N points) is the product $W_1 W_2 \dots W_N$, to be denoted by $\mathcal{W}_N$. The quantity whose variation with distance is to be studied, in the present context of sequential sampling, is $\mathcal{W}_N$; on universality grounds, it is expected to decay with the same correlation length as P_N of Eq. (4).

For strips of widths $L = 4, \dots 11$ at $p = 0.592745$, the best numerical estimate of the appropriate percolation threshold to our knowledge [10], we have generated large numbers (N_{samp}) of independent connected configurations between the origin and column N_0. The weights of the N_{samp} configurations up to respectively columns $N_0 - \Delta$ and N_0 were summed to produce the estimates $\overline{\mathcal{W}}_{N_0-\Delta} = (\sum_{k=1}^{N_{samp}} \mathcal{W}^{(k)}_{N_0-\Delta})/N_{samp}$ and $\overline{\mathcal{W}}_{N_0} = (\sum_{k=1}^{N_{samp}} \mathcal{W}^{(k)}_{N_0})/N_{samp}$. An estimate of the correlation length is then given by

$$\frac{\Delta}{\xi} = -\ln\left(\frac{\overline{\mathcal{W}}_{N_0}}{\overline{\mathcal{W}}_{N_0-\Delta}}\right) \quad . \tag{5}$$

Finally, we have repeated the process n_s times with distinct random-number sequences, in order to estimate fluctuations. We used $N_{samp} = 10^5$, $N_0 = 20$, $\Delta = 10$, $n_s = 100$. Our results are displayed in Table 1, in the form of estimates for the critical decay-of-correlations exponent η, through the identity $\eta = L/\pi\xi(p_c)$ given by conformal invariance [11]. These are to be compared with those, also in Table 1, obtained from the largest eigenvalue of the TM. The values of N_0 and Δ were chosen bearing in mind that, both from general finite-size scaling ideas and from previous results for percolation [1], it is known that the correlation length at criticality must be of order L. The convergence of finite-width results towards the value given by conformal invariance [11], $\eta = 5/24 = 0.208333\dots$ has been investigated elsewhere [12]. For our present purposes the relevant comparison is between the columns of Table 1, which shows

the soundness of the proposed scheme. As expected from the theory of normal distributions, fluctuations shrink with $(N_{samp})^{-1/2}$, because it is there that the accumulation of sample weights leading to self-averaging takes place, but remain approximately constant with n_s. The amount of computational time involved is linearly proportional to $n_s \times N_{samp}$, thus one can produce more accurate results by increasing N_{samp} while reducing n_s to one; in this limit, the width of the error bar for the single (presumably very precise) central estimate can be extrapolated from those obtained for large n_s and correspondingly smaller N_{samp}, via the $(N_{samp})^{-1/2}$ dependence. Since our goal here is to demonstrate the feasibility of the proposed approach, rather than refining numerical values, we did not pursue this line systematically.

We now show results for finite-size conductivity $\sigma_L(p_c)$ at the percolation threshold of a resistor-insulator network. From finite-size scaling, this is expected to vary with strip width as

$$\sigma_L(p_c) \sim L^{-t/\nu} \quad , \tag{6}$$

where the best available estimate for the exponent is $t/\nu = 0.9745 \pm 0.0015$ [6]. We have generated samples of site-diluted resistor networks (where a bond is a resistor if it connects two occupied sites, and an insulator otherwise), according to the procedure delineated above. Now, since the quantity to sample (average conductivity per bond) is naturally accumulated as one proceeds along the strip (instead of decaying exponentially, as is the case with connection probabilities), one does not have to be concerned with weights: it suffices to generate very long samples, and each column configuration will come up with its good weight.

Conductivities have been calculated by Fogelholm's node deletion algorithm [13]. This is very efficient on a strip geometry since it depends on keeping track only of at most $L(L-1)/2$ links among sites, plus $2L$ links to the origin.

Table 2 shows our data for $L = 3$–11 where for each strip width 100 independent samples, each of length 10^5 columns, were generated. Error bars reflect deviations among different samples. A least-squares fit to a log-log plot of the data in Table 2 gives $t/\nu = 1.005 \pm 0.002$, with an accumulated χ^2 per degree of freedom (DOF) = 1.0, an estimate which is 3% above the accepted value [6], with apparently non-overlapping error bars. Before accepting this at face value, some remarks are in order.

Firstly, we perform a similar fit to the resistivity (ρ_L) data on the site superconductivity problem, shown in Table I of Ref. [6]. In $d = 2$ the superconducting exponent s/ν in $\rho_L \sim L^{-s/\nu}$ is the same as t/ν, by duality (see Refs. [5,6]). Also, the same (periodic) boundary conditions across the strip were used there, as opposed to free ones for previous conductivity studies [4]. This is important when one wishes to compare purely finite-size effects between two sets of data. Those authors simulated strips 10^4 times as long as we did, thus the fact that their error bars are two orders of magnitude smaller than our own indicates that both methods have the same intrinsic accuracy. We then turn to comparison of systematic errors. For the *same* range $3 \leq L \leq 11$, the data of Ref. [6] give $t/\nu \simeq 0.913$, though with a very large χ^2/DOF which partly reflects the greater accuracy of individual data in Ref. [6], as well as the need to take corrections to scaling into account. Assuming a power-law correction with exponent ω, always for $3 \leq L \leq 11$, fits of $\rho_L L^{t/\nu}$ to $a + b/L^{\omega}$ for $0.94 \leq t/\nu \leq 1.02$ show that χ^2/DOF indeed has a minimum value at $t/\nu \sim 0.982$–0.987 when ω is kept constant at $1.2 - 1.4$ (see Ref. [6]). The amplitude b varies monotonically between -0.1 and -0.6. A similar analysis of our own data shows that χ^2/DOF has a gentle maximum at $t/\nu \sim 0.95$ and a minimum at $t/\nu \sim 1.025$. The amplitude b starts from 0.44 at $t/\nu = 0.94$ and decreases monotonically, crossing zero at $t/\nu \sim 1.005$. Varying ω along a wider interval, between 1 and 2.5, does not produce any significant change.

Thus, for similar strip widths and comparable amounts of computational effort, our method generates data of comparable quality to other authors'. It seems that for critical conductivity studies in two dimensions one has to reach very large widths, of order 40 sites [4–6], before asymptotic behaviour sets in. While this could be done in Refs. [4–6], the nature of the present algorithm is such that the exponential growth, with strip width, of the number of configurations to be stored is the main obstacle to going further than $L = 11$. However, from past experience [8] we expect such upper limit not to be as stringent for *e.g.* diluted magnets.

We have also studied resistor networks for very low impurity (insulator) concentrations $(1-p)$, where it has been predicted [14] that conductivity must vary as

$$\sigma(p)/\sigma(1) = 1 - \pi(1-p) + \pi(1-p)^2/2 \quad . \tag{7}$$

By using finite-size considerations pertaining to low concentrations of impurities in a cylindrical geometry, we have shown that the finite-size conductivity is

$$\sigma_L(p) = \sigma_\infty(p) + a(p)/L^2 + O(1/L^4) \quad , \tag{8}$$

where $\sigma_\infty(p)$ is given by Eq. (7) and $a(p) = -(1-p)\pi^3/6$. Our data for the normalised conductivity at $p = 0.999$ (where Eq. (8) gives $\sigma_\infty(p) = 0.99686\ldots$ and $a(p) = -5.17 \times 10^{-3}$) and $3 \leq L \leq 11$ are shown in Table 3, where for each strip width 100 independent samples, each of length 10^5 columns, were generated. Error bars reflect deviations among different samples. A least-squares fit of our finite-size data gives $\sigma_\infty = 0.99685 \pm 0.00005$, where the small error bar reflects the fit's overall smoothness, and $a = (-6.0 \pm 1.7) \times 10^{-3}$, in very good agreement with the theoretical prediction.

We have proposed and illustrated a straightforward scheme for diluted systems, in which a transfer-matrix approach can be implemented without giving rise to longitudinal disconnections along a strip. Previous treat-

ments either were restricted to the calculation of the decay of connection probability [1], or could be carried out independent of disconnections, owing to particular geometric [4] or physical [5,6] features, or else were forced to rely on essentially uncontrollable assumptions on the commutation of TMs associated to distinct dilution configurations [8]. Extensions of the present work to dilute magnets [7,8] are now being considered. Further applications would be to the anomalous thermal behaviour of Fe(110) submonolayers on W(110) [15], and to frustrated percolation [16], a problem related to glass-formation processes.

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TABLE I. Estimates of $\eta = L/\pi\xi(p_c)$ at $p = 0.592745$; averages over $n_s = 100$ distinct sequences, each of $N_{samp} = 10^5$ accumulated weights .

L	η (this work)	η (TM)
4	0.21255 ± 0.00020	0.2125576128
5	0.21142 ± 0.00026	0.2114673276
6	0.21069 ± 0.00029	0.2107370714
7	0.21016 ± 0.00039	0.2102232886
8	0.20979 ± 0.00043	0.2098564767
9	0.20954 ± 0.00044	0.2095868033
10	0.20930 ± 0.00047	0.2093833099
11	0.20915 ± 0.00055	0.2092261631

TABLE II. Estimates of $\sigma_L(p_c)$ at $p = 0.592745$; averages over $n_s = 100$ distinct strips, each of length 10^5 columns .

L	σ_L
3	0.34435 ± 0.00063
4	0.25931 ± 0.00054
5	0.20718 ± 0.00053
6	0.17241 ± 0.00047
7	0.14749 ± 0.00045
8	0.12881 ± 0.00038
9	0.11431 ± 0.00042
10	0.10271 ± 0.00035
11	0.09323 ± 0.00033

TABLE III. Estimates of $\sigma_L(p)$ at $p = 0.999$; averages over $n_s = 100$ distinct strips, each of length 10^5 columns. Extr.: extrapolation against $1/L^2$ (see text). Expected: Eq. (7).

L	σ_L
3	0.99618 ± 0.00019
4	0.99648 ± 0.00016
5	0.99661 ± 0.00013
6	0.99669 ± 0.00012
7	0.99673 ± 0.00011
8	0.996753 ± 0.000099
9	0.996775 ± 0.000099
10	0.996791 ± 0.000095
11	0.996804 ± 0.000092
Extr.	0.99685 ± 0.00005
Expected	$0.99686\ldots$